Advanced Python for Scientific Computing

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Follow along!

https://www.msi.umn.edu/content/programming

Or copy files from:

/home/support/public/tutorials/PythonSciComp/

To get the most out of this…

- Basic knowledge of Python
- Working Python install (feel free to use ours!)
  - Enthought Python Distribution / Canopy provides scientific and math libraries pre-installed

```
%  module load python-epd
%  ipython
```

- MSI login + SSH or NX
- **Follow along!**

```
% isub -X  OR  % ssh -X username@itasca.msi.umn.edu
% module load python-epd
% ipython
```


Why Python for Scientific Computing?

- **Rapid development**
  - Easy, readable syntax
  - Versatile tools for experimentation/learning
  - Comprehensive libraries
- **Powerful Features**
  - Process data at near "native code" speeds
  - Excellent visualization packages
  - Comprehensive libraries

When you leave today, you should be able to…

- Program interactively with **ipython**
- understand the basics of **numpy and scipy**
- **Efficiently compute** with large arrays of data
- Load and save data to/from **files on disk**
- Use **matplotlib** to plot data
- Take advantage of supercomputing resources with **parallel computing**
- **Know where to turn** for more help with these topics

Details

- We are describing Enthought Python Distribution.
  - Essentially: Pre-assembled compilation of Python 2.7 + numpy, scipy, other useful libraries
  - Free for academic use, a basic version is free for non-commercial use
  - Your computers, departments, etc may have a different version of Python installed. Everything we will see today is open source.

- In MSI: **module load python-epd**

Workshop Conventions

- UNIX shell commands are indicated with the **percent** sign.
- IPython interpreter commands have In/Out labels
- Neither sign indicates python code that should be entered into a text file.

```
%  module load python-epd
%  ipython
```

```
In [1]: numpy.arange(5)
Out[1]: array([0, 1, 2, 3, 4])
```

```
x = 5
y = 6
print x + y
```

IPython: Interactive Python

- Powerful environment for interactive work
- Run as “ipython” from any terminal
- --pylab option auto-loads **numpy**, sets up graphics for plotting
- Inspect any object with “?” or help()

```
%  module load python-epd
%  ipython --pylab
```

```
In [2]: x = [1,2,3]

In [3]: x?
Type:        list
String Form:[1, 2, 3]
Length:      3
Docstring:
list() -> new empty list
list(iterable) -> new list
initialized from iterable's
items
```

IPython: Interactive Python

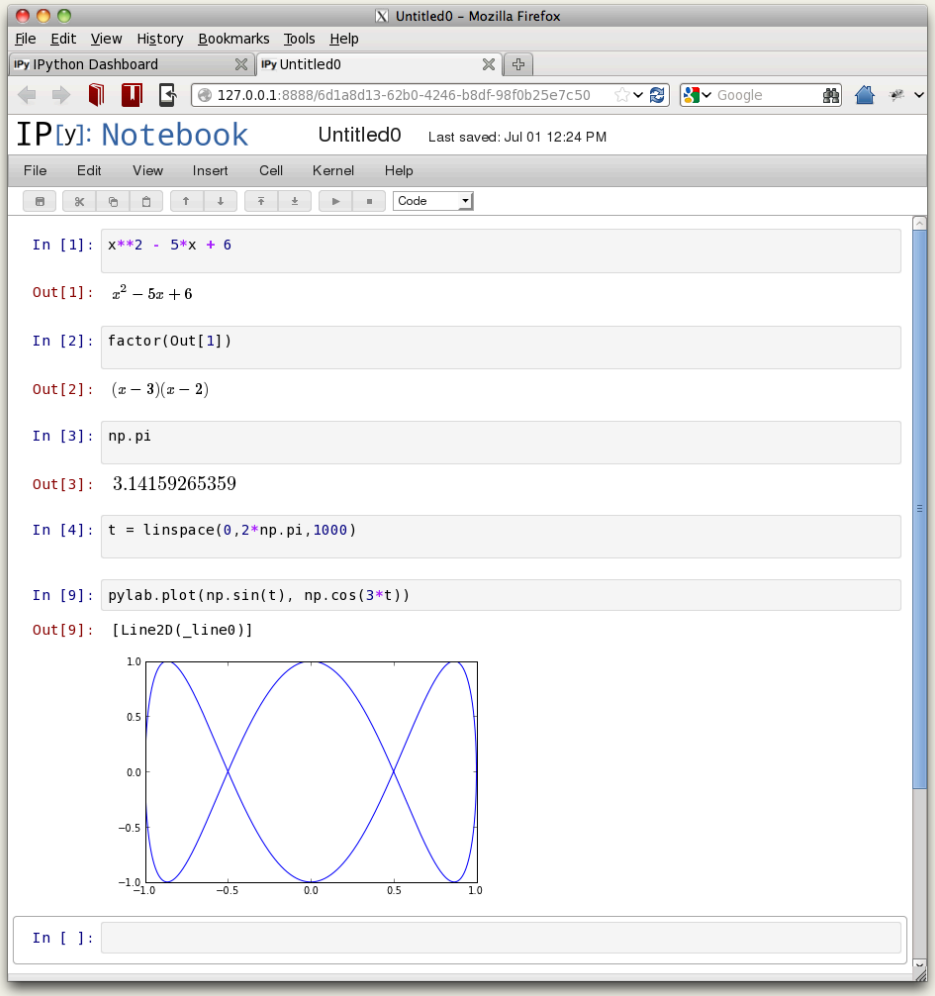
- Build up a workspace of objects and functions
- Full history access through Out[], %recall, up/down arrow keys
- %load, %edit, or %run external files
- Lots more, type %magic

```
In [5]: def df(a,b):
   ....:     return a - b
   ....:

In [6]: df(5,2)
Out[6]: 3

In [7]: Out[6] * 2
Out[7]: 6
```

IPython notebook

- **notebook** creates graphical log in a browser
- Full power of an Ipython session
- You can follow along with most of today's examples in the notebook
- In a command line find where you put the .ipynb files from the examples and type:

```
cd <examples location>
ipython notebook
```



NumPy and SciPy

- **NumPy** provides:
  - the basic array and matrix data types
  - Efficient implementations of low-level math operations
  - A large library of high-level math functions built from efficient primitives
- **SciPy** provides:
  - A home for a wide variety of open-source mathematical and scientific algorithms
  - Modules for optimization, signal processing, linear algebra, statistics, interpolation, and more

NumPy arrays

- Array data type with vectorized operations(similar to Matlab or IDL)
- Supports same operations as Python list type
- …except every element is of same data type
- …so they can be stored in memory packed like C arrays

```
In [9]: a = arange(5)

In [10]: a
Out[10]: array([0, 1, 2, 3, 4])

In [11]: b = ones(5)

In [12]: b
Out[12]: array([ 1.,  1.,  1.,
1.,  1.])

In [13]: a - b * 3
Out[13]: array([-3., -2., -1.,
0.,  1.])

In [14]: sorted(a - b * 3)
Out[14]: [-3.0, -2.0, -1.0,
0.0, 1.0]

In [15]: b.dtype
Out[15]: dtype('float64’)
```

NumPy arrays are fast

addition.py

```
import numpy

def py_add(a, b):
    c = []
    for i in xrange(0,len(a)):
        c.append(1.324 * a[i] -
          12.99 * b[i] + 1)
    return c

def np_add(a, b):
    return 1.324 * a - 12.99 *  b + 1
```

```
In [26]: from addition import *

In [27]: a = arange(1e6)

In [28]: b = random.randn(1e6)

In [29]: len(a)
Out[29]: 1000000

In [30]: %timeit py_add(a,b)
1 loops, best of 3: 2.97 s per loop

In [31]: %timeit np_add(a,b)
100 loops, best of 3: 10 ms per loop
```

Here we are comparing a “pure Python” loop to the equivalent in numpy

Multidimensional arrays

- NumPy arrays are rectangles in arbitrarily many dimensions
- + - * / operate element-by-element for same-shape arrays

```
In [4]: M = arange(2*4*3).reshape([2,4,3])

In [5]: M
Out[5]:
array([[[ 0,  1,  2],
        [ 3,  4,  5],
        [ 6,  7,  8],
        [ 9, 10, 11]],

       [[12, 13, 14],
        [15, 16, 17],
        [18, 19, 20],
        [21, 22, 23]]])

In [6]: M[0,2,2]
Out[6]: 8
```

Array slicing

- Index notation gives access to any "slice" of an array
- Array slices can be assigned – this changes the original array
- X = M[1,:,:].copy() would avoid changing M

```
In [20]: M[1,:,:]
Out[20]:
array([[12, 13, 14],
       [15, 16, 17],
       [18, 19, 20],
       [21, 22, 23]])

In [21]: x = M[1,:,:]

In [22]: x -= 10

In [23]: M
Out[23]:
array([[[ 0,  1,  2],
        [ 3,  4,  5],
        [ 6,  7,  8],
        [ 9, 10, 11]],

       [[ 2,  3,  4],
        [ 5,  6,  7],
        [ 8,  9, 10],
        [11, 12, 13]]])
```

Other common methods

- Numpy arrays have many useful built-in methods

```
In [40]: M = arange(1,10)

In [41]: M.min()
Out[41]: 1

In [42]: M.mean()
Out[42]: 5.0

In [43]: M.max()
Out[43]: 9

In [44]: M.sum()
Out[44]: 45

In [45]: M.prod()
Out[45]: 362880

In [46]: M.ptp()
Out[46]: 8

In [47]: M.cumsum()
Out[47]: array([ 1,  3,  6, 10, 15, 21, 28, 36, 45])
```

Other common methods

- …and the numpy module provides more

```
In [50]: numpy.floor(M)
Out[50]: array([ 1.,  2.,  3.,  4.,  5.,  6.,  7.,  8.,
9.])

In [51]: numpy.diff(M)
Out[51]: array([1, 1, 1, 1, 1, 1, 1, 1])

In [52]: numpy.dot(M,M)
Out[52]: 285

In [54]: numpy.sin(M)
Out[54]:
array([ 0.84147098,  0.90929743,  0.14112001,
-0.7568025 , -0.95892427,
   -0.2794155 ,  0.6569866 ,  0.98935825,  0.41211849])

In [56]: numpy.log(M)
Out[56]:
array([ 0.        ,  0.69314718,  1.09861229,
1.38629436,  1.60943791,
    1.79175947,  1.94591015,  2.07944154,  2.19722458])
```

Conditions and tests

- Vectorized logical operators + indexing functions
- Output of index functions can be used to slice arrays

```
In [57]: C = arange(10)

In [58]: C
Out[58]: array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])

In [59]: C == 5
Out[59]: array([False, False, False, False, False,
True, False, False, False, False], dtype=bool)

In [60]: numpy.where(C == 5)
Out[60]: (array([5]),)

In [67]: numpy.where((C > 3) & (C < 7))
Out[67]: (array([4, 5, 6]),)

In [72]: C[numpy.where((C > 3) & (C < 7))]
Out[72]: array([4, 5, 6])
```

Conditions and tests

- Vectorized logical operators + indexing functions
- Output of index functions can be used to slice arrays

```
In [73]: x = linspace(0,2*pi,100)

In [74]: y = sin(x)

In [75]: x[where(y > 0.9)]
Out[75]:
array([ 1.14239733,  1.20586385,  1.26933037,
        1.33279688,  1.3962634 ,
        1.45972992,  1.52319644,  1.58666296,
        1.65012947,  1.71359599,
        1.77706251,  1.84052903,  1.90399555,
        1.96746207])
```

More useful numpy modules

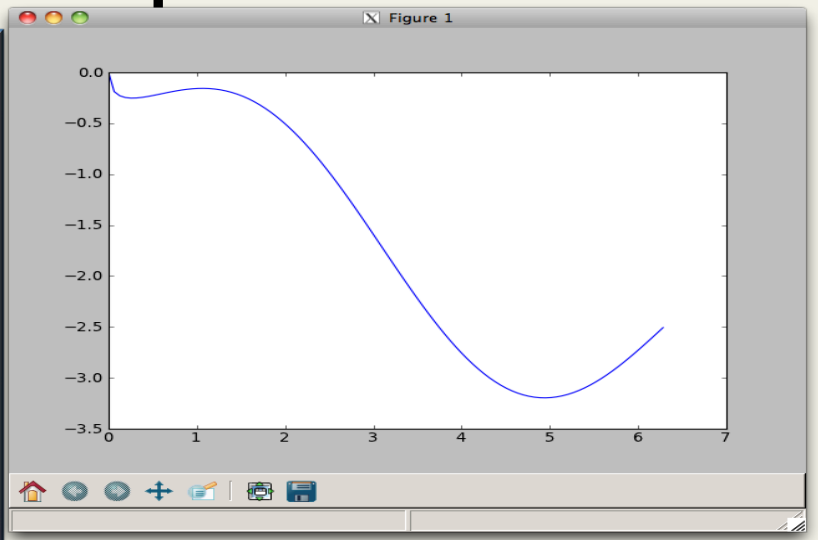
- **numpy.fft** – FFTs, forward/inverse, 1-D and N-D
- **numpy.random** – generate random numbers, many distributions to choose from
- **numpy.matrix** – special arrays that obey matrix math
- **numpy.polynomial** – module for representing and manipulating arbitrary polynomials

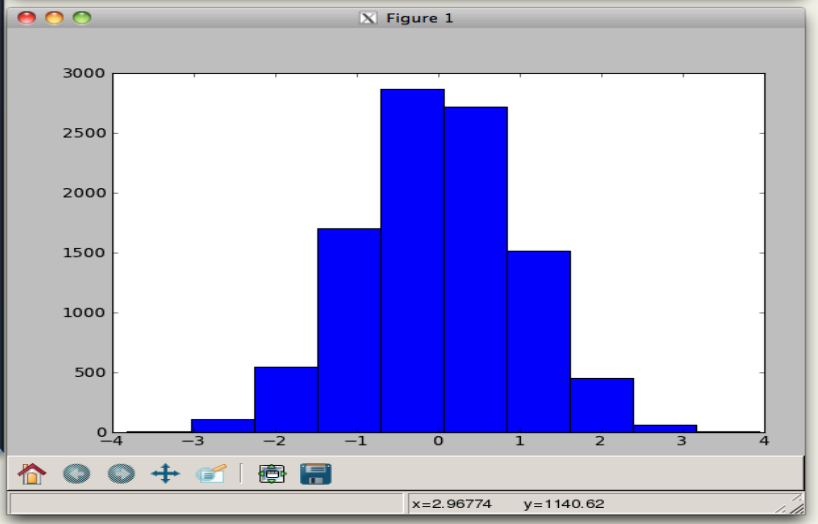
Plotting made easy

- **Matplotlib** provides high-quality 2-D (and some 3-D) plotting
  - Display in window or output to PDF, SVG, PNG, etc
  - Implemented as modular object-oriented system
- **Pylab** provides a Matlab-ish interactive interface to Matplotlib
  - Access with ipython --pylab
  - Defaults to popping up plots in a separate window

Some basic examples…

```
% ipython --pylab

In [1]: x =linspace(0,2*pi,100)

In [2]: y = sin(x)

In [3]: plot(x, sin(x) - sqrt(x))
Out[3]: [<matplotlib.lines.Line2D at 0x3995b90>]

In [4]: t = random.randn(10000)

In [5]: hist(t, 10)
Out[5]:
(array([   9,  110,  548, 1704, 2864, 2717,
1519,  457,   65,    7]),
 array([-3.81576343, -3.04011185, -2.26446028,
-1.4888087 , -0.71315713,
        0.06249445,  0.83814602,  1.61379759,
2.38944917,  3.16510074,
        3.94075232]),
 <a list of 10 Patch objects>)
```





Some advanced examples…

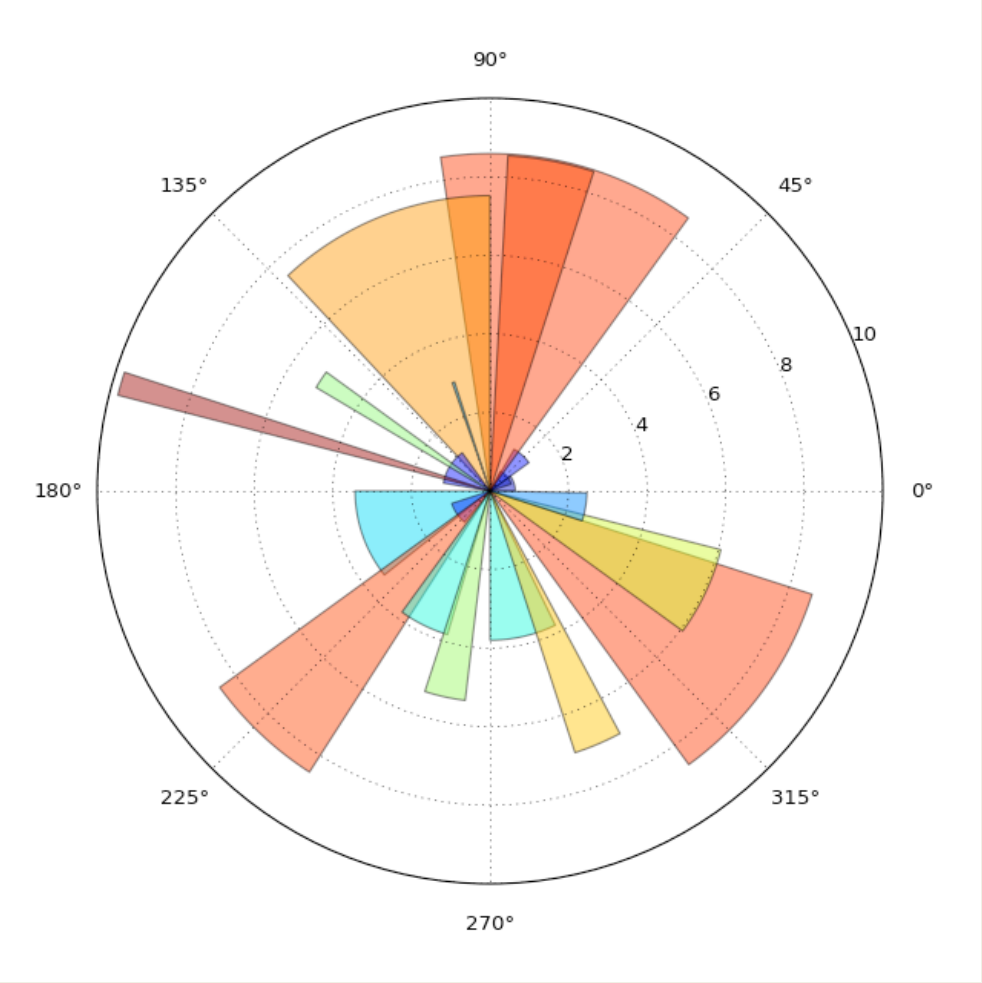
- These examples are from the **matplotlib.org** examples section…

Some advanced examples…

plot-polarbars.py

```
import numpy as np
import matplotlib.cm as cm
from matplotlib.pyplot import figure, show, rc

# force square figure and square axes looks better for polar, IMO
fig = figure(figsize=(8,8))
ax = fig.add_axes([0.1, 0.1, 0.8, 0.8], polar=True)

N = 20
theta = np.arange(0.0, 2*np.pi, 2*np.pi/N)
radii = 10*np.random.rand(N)
width = np.pi/4*np.random.rand(N)
bars = ax.bar(theta, radii, width=width, bottom=0.0)
for r,bar in zip(radii, bars):
    bar.set_facecolor( cm.jet(r/10.))
    bar.set_alpha(0.5)

show()
```

Some advanced examples…

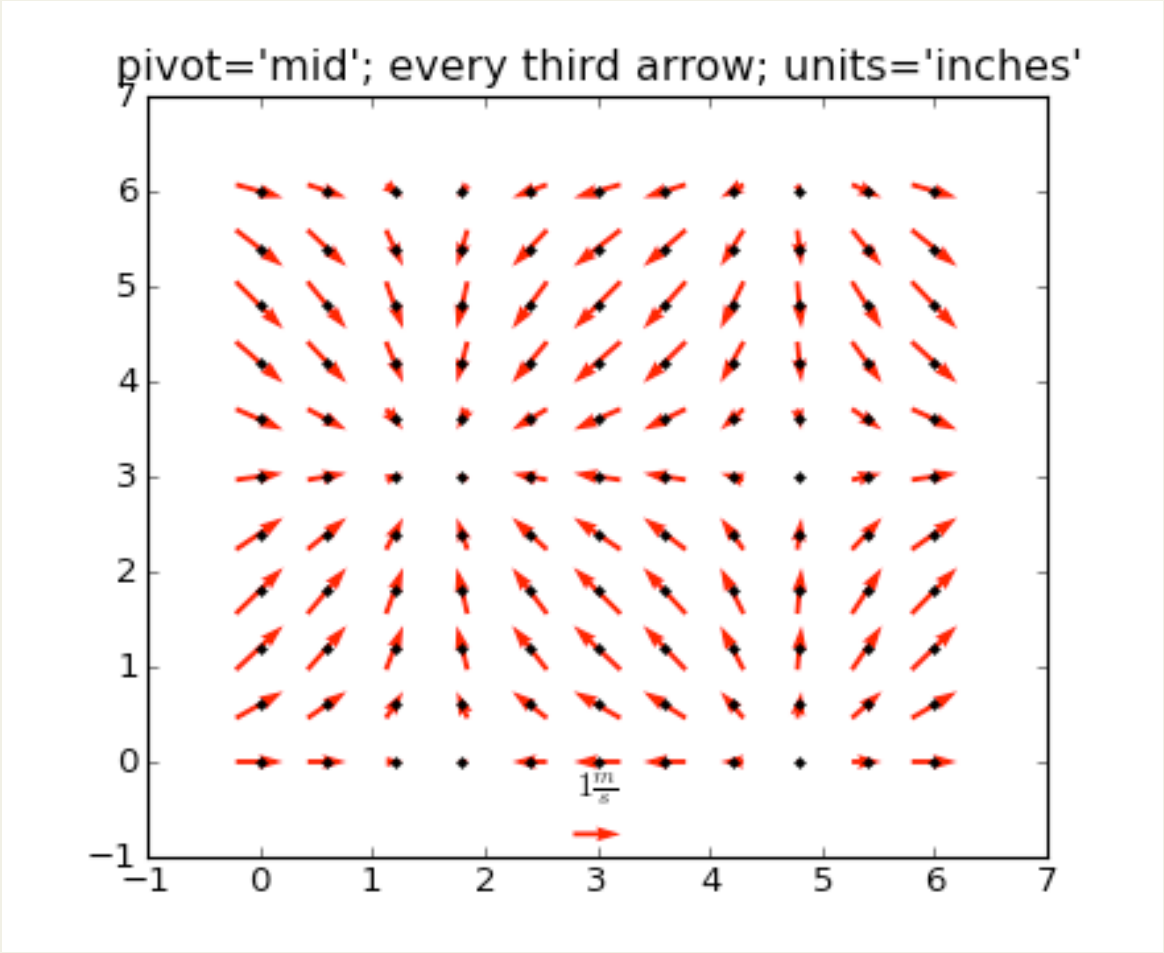


Some advanced examples…

plot-vectors.py

```
import numpy as np
from pylab import *
from numpy import ma
X,Y = meshgrid( arange(0,2*pi,.2),arange(0,2*pi,.2) )
U = cos(X)
V = sin(Y)

figure()
Q = quiver( X[::3, ::3], Y[::3, ::3], U[::3, ::3], V[::3, ::3],
                  pivot='mid', color='r', units='inches' )
qk = quiverkey(Q, 0.5, 0.03, 1, r'$1 \frac{m}{s}$',
                  fontproperties={'weight': 'bold'})
plot( X[::3, ::3], Y[::3, ::3], 'k.')
axis([-1, 7, -1, 7])
title("pivot='mid'; every third arrow; units='inches'")
show()
```

Some advanced examples…

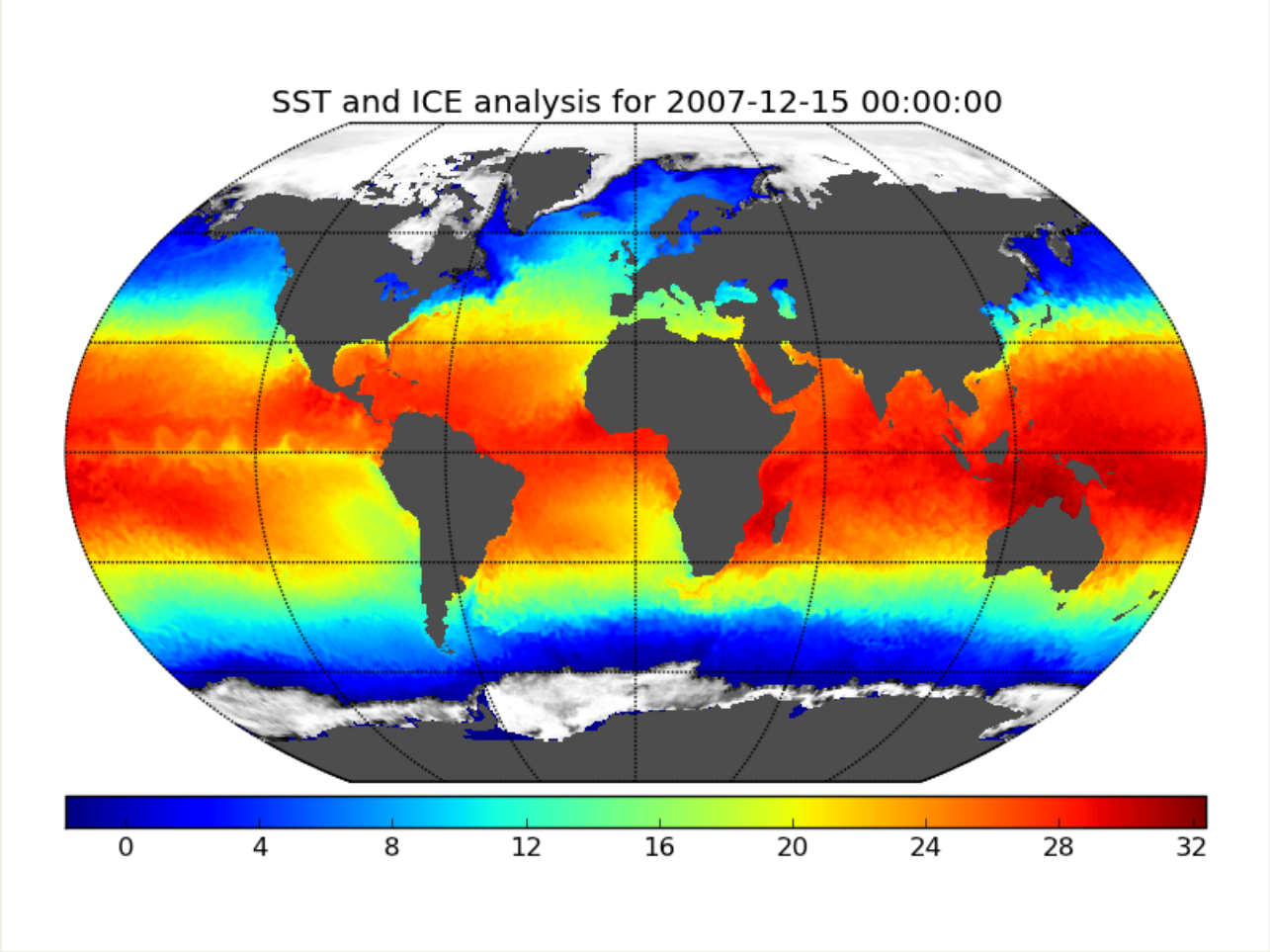


Some advanced examples…

plot-icemap.py

```
from mpl_toolkits.basemap import Basemap
from netCDF4 import Dataset, date2index
import numpy as np
import matplotlib.pyplot as plt
from datetime import datetime
date = datetime(2007,12,15,0)
dataset = Dataset('http://www.ncdc.noaa.gov/thredds/dodsC/OISST-V2-AVHRR_agg')
timevar = dataset.variables['time']
timeindex = date2index(date,timevar)
sst = dataset.variables['sst'][timeindex,:].squeeze()
ice = dataset.variables['ice'][timeindex,:].squeeze()
lons, lats = np.meshgrid(dataset.variables['lat'][:] , dataset.variables['lon'][:] )
ax = plt.figure().add_axes([0.05,0.05,0.9,0.9])
m = Basemap(projection='kav7',lon_0=0,resolution=None)
m.drawmapboundary(fill_color='0.3')
im1 = m.pcolormesh(lons,lats,sst,shading='flat',cmap=plt.cm.jet,latlon=True)
im2 = m.pcolormesh(lons,lats,ice,shading='flat',cmap=plt.cm.gist_gray,latlon=True)
m.drawparallels(np.arange(-90.,99.,30.))
m.drawmeridians(np.arange(-180.,180.,60.))
cb = m.colorbar(im1,"bottom", size="5%", pad="2%")
ax.set_title('SST and ICE analysis for %s'%date)
plt.show()
```

Some advanced examples…



SciPy expands the menu

- Clustering algorithms (scipy.cluster)
- Integration and ODEs (scipy.integrate)
- Interpolation (scipy.interpolate)
- Input and output (scipy.io)
- Linear algebra (scipy.linalg)
- Multi-dimensional image processing (scipy.ndimage)
- Optimization and root finding (scipy.optimize)
- Signal processing (scipy.signal)
- Sparse matrices (scipy.sparse)
- Spatial algorithms and data structures (scipy.spatial)
- Special functions (scipy.special)
- Statistical functions (scipy.stats)
- And then some…

SciPy is also fast

- Most SciPy routines use fast NumPy low-level math operations
- Some SciPy routines use highly optimized external libraries
  - E.g. scipy.linalg links to BLAS, LAPACK or MKL behind the scenes

Data on disk

- Chances are you want to load and save data
- **numpy** and **scipy.io** offer a variety of facilities

Data on disk: text files

- **Very common for smaller data sets:** simple columns of numbers
- numpy.loadtxt() – simple interface, good defaults
- numpy.genfromtxt() – more complex, handles unusual formatting, comments, missing values, etc

```
data.txt

0.000 10.000 20.000 30.000 40.000
1.000 11.000 21.000 31.000 41.000
2.000 12.000 22.000 32.000 42.000
3.000 13.000 23.000 33.000 43.000
4.000 14.000 24.000 34.000 44.000
…
```

```
In [21]: A = numpy.loadtxt('data.txt')

In [22]: A
Out[22]:
array([[  0.,  10.,  20.,  30.,  40.],
       [  1.,  11.,  21.,  31.,  41.],
       [  2.,  12.,  22.,  32.,  42.],
       [  3.,  13.,  23.,  33.,  43.],
…
```

Data on disk: text files

- Numpy.savetxt() – write to columns of numbers

```
In [25]: numpy.savetxt('data.txt', A, delimiter=",",
                       fmt="%3.3f")

In [26]: %pycat data.txt
0.000,10.000,20.000,30.000,40.000
1.000,11.000,21.000,31.000,41.000
2.000,12.000,22.000,32.000,42.000
3.000,13.000,23.000,33.000,43.000
4.000,14.000,24.000,34.000,44.000
5.000,15.000,25.000,35.000,45.000
6.000,16.000,26.000,36.000,46.000
7.000,17.000,27.000,37.000,47.000
8.000,18.000,28.000,38.000,48.000
9.000,19.000,29.000,39.000,49.000
```

Data on disk: binary formats

- **Binary data** is much more scalable
  - Smaller files on disk
  - Faster to load and save
  - May be necessary to exchange data with other software
  - Stick to **portable** (machine-independent) formats

Data on disk: binary formats

- **NumPy native format (.npy)**
  - numpy.load() and numpy.save()
  - Or use numpy.savez() to store many arrays in compressed .npz
  - Fast, portable, but mostly only supported by Python
- **scipy.io.matlab** – support for Matlab (.mat)
  - scipy.io.loadmat() and scipy.io.savemat()
- **scipy.io.idl** – read (no save) IDL .sav files
  - scipy.io.readsav()

Data on disk: binary formats

- **Many standard formats supported**
  - scipy.io.netcdf – NetCDF3 interface
  - h5py exposes HDF5 API
  - PyTables is an excellent high-level interface to HDF5
  - pyfits for FITS datasets
  - Etc…

Scaling up with parallelization

- For big jobs you will eventually want to **parallelize** your code
- The Python interpreter has trouble with multithreading – multi-process is usually best
- Approach depends on the problem you need to solve

Parallel processes

- Many jobs need to process lots of data, don't need to communicate amongst themselves
- Sometimes called "embarrassingly parallel"
- **GNU Parallel** -- a simple way to launch jobs
  - Launch one job for every file in a dir, line in a file, etc
  - Can work with PBS on itasca to use many nodes

GNU Parallel example

```
% ssh itasca
% qsub -I -l walltime=00:05:00,pmem=1000mb,nodes=10:ppn=8
qsub: waiting for job 616263.node1081.localdomain to start
qsub: job 616263.node1081.localdomain ready

% module load parallel
% module load python-epd
% seq 80 | parallel -j 8 --sshloginfile $PBS_NODEFILE --env PATH 'echo Job {} on $(hostname)'
Job 1 on node0109
Job 2 on node0109
Job 3 on node0109
Job 4 on node0109
Job 5 on node0109
Job 6 on node0109
Job 7 on node0109
Job 8 on node0109
Job 9 on node0080
Job 10 on node0080
Job 11 on node0080
Job 12 on node0080
... Etc . . .
```

GNU Parallel example

- -j should match ppn (unless you know what you're doing) – this is processes per node
- Will run one job per line of input on stdin or in argfile – max of nodes * ppn running at once
- See "man parallel" for more features

```
Alternate ways to run parallel:

% parallel –a <argfile> -j 8 --sshloginfile $PBS_NODEFILE
      --env PATH 'echo Job {} on $(hostname)'

# Load any needed modules from a shell script:
% parallel –a <argfile> -j 8 --sshloginfile $PBS_NODEFILE "myscript.sh {}"
```

multiprocessing module

- Built in to python standard library: **multiprocessing**
- Easily spawn new copies of python to execute code
- Works best with multiple cores on single machine
- Some restrictions on your code:
  - Uses pickle to communicate to other processes, may be slow to transfer giant data structures
  - Transfers your python code as well, you cannot use lambda functions in any classes that worker processes will use

Simple multiprocessing example

- Process some letters and sleep in a pool:

```
import multiprocessing
import time

data = ( ['a', '2'], ['b', '4'], ['c', '6'], ['d', '8'], ['e', '1'],
['f', '3'], ['g', '5'], ['h', '7'] )

def mp_worker((inputs, the_time)):
    print " Processs %s\tWaiting %s seconds" % (inputs, the_time)
    time.sleep(int(the_time))
    print " Process %s\tDONE" % inputs

def mp_handler():
    p = multiprocessing.Pool(2)
    p.map(mp_worker, data)

mp_handler()
```

MPI for Python

- MPI "Message Passing Interface" enables parallel processes to communicate efficiently
- Commonly one process will be "controller" and manage worker processes
- Inherent support for scatter-gather operations
- MPI is well-supported on our clusters
- mpi4py interfaces to MPI from inside Python
- Caveat for MPI gurus: numpy does not have distributed arrays yet, complicates some algorithms

Example with mpi4py

- Simple “Hello world” script

```
Helloworld-mpi.py

#!/usr/bin/env python
"""
Parallel Hello World
"""

from mpi4py import MPI
import sys

size = MPI.COMM_WORLD.Get_size()
rank = MPI.COMM_WORLD.Get_rank()
name = MPI.Get_processor_name()

sys.stdout.write(
    "Hello, World! I am process %d of %d on %s.\n"
    % (rank, size, name))
```

Example with mpi4py

- Simple “Hello world” script

```
% ssh itasca
% qsub -I -l walltime=00:05:00,pmem=1000mb,nodes=10:ppn=8
qsub: waiting for job 616294.node1081.localdomain to start
qsub: job 616294.node1081.localdomain ready

% module load python-epd
% mpirun python helloworld-mpi.py
Hello, World! I am process 3 of 80 on node0079.
Hello, World! I am process 52 of 80 on node0126.
Hello, World! I am process 6 of 80 on node0079.
Hello, World! I am process 25 of 80 on node0099.
Hello, World! I am process 14 of 80 on node0080.
Hello, World! I am process 64 of 80 on node0128.
. . . Etc . . .
```

More with mpi4py

- Possible to pass numpy arrays like buffers

```
comm = MPI.COMM_WORLD
rank = comm.Get_rank()

# pass explicit MPI datatypes
if rank == 0:
  data = numpy.arange(1000, dtype='i')
  comm.Send([data, MPI.INT], dest=1, tag=77)
elif rank == 1:
  data = numpy.empty(1000, dtype='i')
  comm.Recv([data, MPI.INT], source=0, tag=77)
```

More with mpi4py

- Also works with (pickle-able) Python objects
  - Much slower than C-based arrays, but very convenient

```
from mpi4py import MPI

comm = MPI.COMM_WORLD
rank = comm.Get_rank()

if rank == 0:
  data = {'key1' : [7, 2.72, 2+3j],
          'key2' : ( 'abc', 'xyz')}
else:
  data = None

data = comm.bcast(data, root=0)
```

Too much to cover…

- **Ipython notebook** – connect to ipython with a browser for a Mathematica-like notebook interface
- **PyCUDA** and **PyOpenCL** – GPU computing
- **SymPy** – Mathematica-style symbolic math
- **Databases** are easy to connect to Python; or use data analytics toolkit like **Pandas** or **PyTables**

Community and Documentation

- Actively developed and supported
- Excellent documentation
- www.python.org/doc
- Scipy.org
- wiki.scipy.org
- Ipython.org
- matplotlib.org
- Mpi4py.scipy.org

Next Step

- Hands-on
- You can also run the examples on your laptop's Python distribution
- Full academic version of Enthought Canopy installed at MSI in labs and on supercomputers
- Questions!